# THEOCHEM, VOLUME 55 (1989)

(*Journal of Molecular Structure, Vol. 186*)

## AUTHOR INDEX


Adamowicz, L., 273
Alcudia, F., 211
Ángyán, J.G., 53, 61

Barbarella, G., 197
Broeker, J.L., 273

Csizmadia, I.G., 1, 53

Daudel, R., 53
Domenicano, A., 185

Eggers, M.D., 69

Fälth, L., 239
Fernández, I., 211
Flakus, H., 117
Fossey, J., 305
Fujihara, H., 261
Furukawa, N., 261

Glass, R.S., 273

Håkansson, U., 239
Harcourt, R.D., 131
Hargittai, I., 185

Iffert, R., 347
Innes, E.A., 1

Jug, K., 347

Kanada, Y., 1
Kucsman, Á., 53

Livant, P.D., 69
Llera, J.M., 211

Mayer, I., 43
McKee, M.L., 69
Mezey, P.G., 117
Minkin, V.I., 293
Minyaev, R.M., 293

Oae, S., 321

Poirier, R.A., 101
Portalone, G., 185

Robinson, E.A., 9, 29
Ruekberg, B.P., 85

Sandström, J., 239
Schultz, G., 185
Sorba, J., 305

Trujillo, M., 211

Volatron, F., 167

Yadav, A., 101
Yadav, V.K., 101
Young, P.R., 85
Yudilevich, J.A., 293

Zorrilla, F., 211

# THEOCHEM, VOLUME 55 (1989)

*(Journal of Molecular Structure, Vol. 186)*

## SUBJECT INDEX


Alkyl radicals
HO and HS substituent effect on alkyl radicals: an ab-initio molecular orbital study, 305
Alkyl transfer reactions
The role of hypervalent intermediates in alkyl transfer reactions at sulfonium centers, 85
Azo species of Si(IV), P(V), S(VI), and Cl(VII)
The duodecet rule. Part 1. Valence bond structures of oxo and azo species of Si(VI), P(V), S(VI), and Cl(VII), 9

Bond orders
Bond orders in three-centre bonds: an analytical investigation into the electronic structure of diborane and the three-centre four electron bonds of hypervalent sulphur, 43
Bond orders in three-centre bonds. Part 2. The role of *d*-orbital participation in sulfuranes and related systems, 61

C=S groups
Interactions between C=S groups in 1,2- and 1,3-*bis* (thiocarbonyl) compounds: a study by spectroscopy, X-ray crystallography, and CNDO/S calculations, 239
Circumambulatory rearrangements
Reaction paths of circumambulatory rearrangements of sulfur-substituted cyclopentadienes, 293
Conjugation
Rotation-independent conjugation of sulfur–nitrogen bonds, 117
Cyclopentadienes
Reaction paths of circumambulatory rearrangements of sulfur-substituted cyclopentadienes, 293

Diborane
Bond orders in three-centre bonds: an analytical investigation into the electronic structure of diborane and the three-centre four-electron bonds of hypervalent sulphur, 43
Dithia dications
Molecular structure of dithia dications and some aspects of their chemistry, 261
1,5-Dithiocane derivatives
Theoretical studies on transannular S–S interactions in geometrically constrained 1,5-dithiocane derivatives, 273
*p*-Dithiolbenzene
The molecular structure of *p*-dithiolbenzene as determined by electron diffraction, 185
Duodecet rule
The duodecet rule. Part 1. Valence bond structures of oxo and azo species of Si(IV), P(V), S(VI), and Cl(VII), 9
The duodecet rule. Part 2. C–H hydrogen bonding by sulfonyl compounds, 29

Electron diffraction
The molecular structure of *p*-dithiolbenzene as determined by electron diffraction, 185

HO and HS substituent effect
HO and HS substituent effect on alkyl radicals: an ab-initio molecular orbital study, 305
Hydroxysulphoxides
Studies on conformation and configuration of β-hydroxysulphoxides, 211
Hypervalent (decet) sulfur compounds
Bonding in selected normal (octet), hypervalent (decet) and super-hypervalent (duodecet) sulfur compounds, 1
Hypervalent intermediates
The role of hypervalent intermediates in

alkyl transfer reactions at sulfonium centers, 85

O
Some periodic trends in organic compounds containing O, S, Se, and Te: an ab initio study, 101
(Octet) sulfur compounds
Bonding in selected normal (octet), hypervalent (decet) and super-hypervalent (duodecet) sulfur compounds, 1
Organic sulfur chemistry
Several unsolved problems of chemical behavior of the sulfur atom in organic sulfur chemistry, 321
Oxo species of Si(IV), P(V), S(VI), and Cl(VII)
The duodecet rule. Part 1. Valence bond structures of oxo and azo species of Si(IV), P(V), S(VI), and Cl(VII), 9
Oxygen-17 nuclear magnetic resonance spectroscopy
Sulfur-33 and oxygen-17 nuclear magnetic resonance spectroscopy of compounds containing -SO- and $-SO_2-$ moieties, 197

Periodic trends
Some periodic trends in organic compounds containing O, S, Se, and Te: an ab initio study, 101

S
Some periodic trends in organic compounds containing O, S, Se, and Te: an ab initio study, 101
S-F
Qualitative valence-bond descriptions of bonding for S-N, S-O, S-F and S-S compounds via increased-valence structures, 131
S-N
Qualitative valence-bond descriptions of bonding for S-N, S-O, S-F and S-S compounds via increased-valence structures, 131
S-O
Qualitative valence-bond descriptions of binding for S-N, S-O, S-F and S-S compounds via increased-valence structures, 131
S-S
Qualitative valence-bond descriptions of bonding for S-N, S-O, S-F and S-S compounds via increased-valence structures, 131
Se
Some periodic trends in organic compounds containing O, S, Se, and Te: an ab initio study, 101
SINDO1 study
SINDO1 study of sulphur isomers and sulphur fluorine compounds, 347
SO- and $-SO_2-$ moieties
Sulfur-33 and oxygen-17 nuclear magnetic resonance spectroscopy of compounds containing -SO- and $-SO_2-$ moieties, 197
Sulfonium centers
The role of hypervalent intermediates in alkyl transfer reactions at sulfonium centers, 85
Sulfonium compounds
Intramolecular sulfur-oxygen interaction in sulfonium compounds and sulfoxides, 53
Sulfonyl compounds
The duodecet rule, Part 2. C-H hydrogen bonding by sulfonyl compounds, 29
Sulfoxides
Intramolecular sulfur-oxygen interaction in sulfonium compounds and sulfoxides, 53
Sulfur atom
Several unsolved problems of chemical behavior of the sulfur atom in organic sulfur chemistry, 321
Sulfur-33 nuclear magnetic resonance spectroscopy
Sulfur-33 and oxygen-17 nuclear magnetic resonance spectroscopy of compounds containing -SO- and $-SO_2-$ moieties, 197
Sulfur-nitrogen bonds
Rotation-independent conjugation of sulfur-nitrogen bonds, 117
Sulfur-oxygen interaction
Intramolecular sulfur-oxygen interaction in sulfonium compounds and sulfoxides, 53
Sulfur-substituted cyclopentadienes
Reaction paths of circumambulatory rearrangements of sulfur-substituted cyclopentadienes, 293
Sulfuranes
Ab initio study of sulfuranes, 69
Bond orders in three-centre bonds. Part 2. The role of *d*-orbital participation in sulfuranes and related systems, 61

Qualitative valence bond analysis of (10-S-4) sulfuranes and (9-S-3) sulfuranyl radicals, 167
Sulfuranyl radicals
Qualitative valence bond analysis of (10-S-4) sulfuranes and (9-S-3) sulfuranyl radicals, 167
Sulphur fluorine compounds
SINDO1 study of sulphur isomers and sulphur fluorine compounds, 347
Sulphur isomers
SINDO1 study of sulphur isomers and sulphur fluorine compounds, 347
Super-hypervalent (duodecet) sulfur compounds
Bonding in selected normal (octet), hypervalent (decet) and super-hypervalent (duodecet) sulfur compounds, 1

Te
Some periodic trends in organic compounds containing O, S, Se, and Te: an ab initio study, 101

1,2- and 1,3-*bis*(Thiocarbonyl)
Interactions between C=S groups in 1,2- and 1,3-*bis*(thiocarbonyl) compounds: a study by spectroscopy, X-ray crystallography, and CNDO/S calculations, 239
Three-centre bonds
Bond orders in three-centre bonds. Part 2. The role of *d*-orbital participation in sulfuranes and related systems, 61
Three-centre four-electron bonds of hypervalent sulphur
Bond orders in three-centre bonds: an analytical investigation into the electronic structure of diborane and the three-centre four-electron bonds of hypervalent sulphur, 43
Transannular S–S interactions
Theoretical studies on transannular S–S interactions in geometrically constrained 1,5-dithiocane derivatives, 273